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Studies on the Relation between the Composition and the Surface States in Binary Alloys

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Considering that the alkyl group is non-polar and polyethylene oxide is a large polar group, it may be reasonable that the dielectric constant ϵ' of PEGAE varied with the lengths of ethylene oxide and methylene chain.

The dielectric constant ϵ' for each sample gradually decreased with increasing the frequency and temperature, but the maximum of the dielectric loss ϵ'' was not found over the present frequency and temperature range. Hence it appears that the critical frequency in the dielectric relaxation of the PEGAE is much higher than 30 Mc.

The author is much indebted to Prof. R. Goto for his interest in this work.

23. Studies on the Relation between the Composition and the Surface States in Binary Alloys

Ken-ichi Fukui and Teijiro Yonezawa

(Kodama Laboratory)

For the binary alloy (composition: atom I: atom II = $m:1$, $n(m+1)$ th atoms from the surface are always the atom II, n is any positive integer) a general equation giving energies of surface states E ,

$$\sin (m+1)\mu_1 (\cos^2 y - 2\cos y \cos \mu_2 + 1) = 2\sin m\mu_1 (\cos \mu_1 - \cos \mu_2),$$

was derived using an assumed one-dimensional well-type periodical potential field, where

$$\cos y = \cos \beta a + (a/\beta) \sin \beta a, \quad a = (-2mE/\hbar^2)^{\frac{1}{2}},$$

$$\cos \mu_1 = \cos \beta a - (P_1/\beta) \sin \beta a, \quad \beta = (2m(E + W_a)/\hbar^2)^{\frac{1}{2}},$$

$$\cos \mu_2 = \cos \beta a - (P_2/\beta) \sin \beta a,$$

P_1, P_2 : constants relating to the area of well,

a : lattice constant,

W_a : potential jump at the surface.

As these states should be exponentially damped on both sides of the surface, we had to add another restriction

$$|\{\cos y \sin(m+1)\mu_1 - \sin m\mu_1\} / \sin \mu_1| < 1.$$

Following conclusions were derived from these equations, taking only the energy range $0 > E > -W_a$ into consideration.

(a) The changes of surface levels with the interior compositions were very small in comparison with the changes with the modification of surface potential curves,

(b) The band in pure metal was separated into $m+1$ pieces in alloy, and the total number of surface states was either $m+2$ or 2.

(c) An attempt of introducing the concept of the surface state into the explanation of activated adsorption had already been made by the authors (1st ann. meet., Chem. Soc. Japan (May 3, 1948)). Considering above results (a) from this standpoint, it may be able to conclude that the change of catalytic activity in alloys depends much upon the various irregularities at the surface, and little upon the "interior" composition.

24. Vapor Phase Catalytic Condensation of Furfural and Acetaldehyde

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Vapor phase condensation of furfural with acetaldehyde in the presence of several basic catalysts were investigated for the purpose of obtaining furfuracrolein.

Using MgO catalyst under the suitable condition, we could obtain furfuracrolein with 70.5% yield for theoretical: some experimental results are tabulated in following 3 tables, where the mol ratio of acetaldehyde to furfural is 1.3. The influence of the mol ratio in charge was also investigated, and the result indicated that in general the yield was larger when furfural was used in excess.

Tab. 1. Comparison of various catalysts.
(350°C: contact time: 24.5 sec)

Catalyst	F · A	R	A/F	k_1/k_2
MgO	0.705	0.047	1.55	2.30
ZnO	0.553	0.033	1.29	1.23
CaO	0.360	0.259	4.14	0.57
K ₂ CO ₃	0.256	0.314	1.31	0.34

F · A: (mol furfuracrolein produced/mol furfural converted)

R: (g resinous matter produced/g total aldehyde used)

A/F: (mol ratio of acetaldehyde to furfural which was converted to resinous matter)

k_1/k_2 : (ratio of rate constant of desired reaction to that of resin formation reaction)

Tab. 2. Influence of temperature.
(Catalyst: MgO; Contact time: 24.5 sec)

Temp. °C	F · A	R	A/F	k_1/k_2
250	0.558	0.047	1.84	1.26
300	0.484	0.126	1.85	0.95
350	0.482	0.104	1.19	0.94
400	0.464	0.082	0.97	0.84